Platform: Systems molecular science

Small molecule discovery colloquium

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Noyori Materials Science Laboratory, 2nd floor, Chemistry Gallery

Protochemometric virtual screening: a launchpad to small molecule discovery and design

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Abstract: Ligand-based virtual screening (LBVS), an alternative to structure-based VS, develops chemical description mathematical models, where compound properties are the independent variables and a single target property such as bioactivity on a specific protein or cell line is modeled as the dependent variable. This technique is effective when the target property under study has been experimentally evaluated with a medium to large size compound library. The resulting model can be used to screen newly designed compounds for bioactivity, thus yielding new starting materials for projects. A setback is that it becomes inapplicable when no prior information is available about a target protein or cellular system.

To remedy this situation, proteochemometric or chemogenomic models have extended the LBVS concept by using two key additions. First, a target protein or system is encoded by a collection of independent variables and appended to the ligand descriptors. Second, many targets or systems are merged together for calculation of a single, and importantly, transductive model. A significant benefit of such an approach is that a single model now has the potential to explore both compound and protein space directions simultaneously. In this talk, I will discuss the practical aspects of the extended proteochemometric approach, provide a demonstration, and hint at the potential of proteochemometrics through its conjunction with other technologies such as next-generation sequencing and peptide synthesis.

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